

# Theoretical studies of quantum entanglement and coherence of many-electron states in nanostructures

## Final Progress Report

### 1 Project Motivation, Objectives, and Methods

#### 1.1 Motivation

Recently, a consensus has been gradually emerging that solid state nanoscale systems may eventually become the most promising prototypes of the future quantum information devices. In a solid state environment, however, the electron correlations are ubiquitous, and often they can not be neglected by any means. Nevertheless, the continuing studies (including those carried out in the framework of this project) have indicated that, instead of being an annoying nuisance to be rid of, the unavoidable interactions in nanoscale systems and the concomitant many-body effects may provide for the new opportunities for constructing novel types of qubits which can enjoy a high degree of intrinsic coherence due to the strongly correlated nature of the underlying many-electron states.

For one, in the presence of a spin-orbit coupling in a conducting crystal which renders spin a non-conserving quantum number, one may consider the still conserved total electron angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  as a better candidate for a robust qubit. Also, considering the difficulty of populating a realistic quantum dot with a single electron, a better chance for constructing a quantum dot-based spin qubit might be offered by the correlated states of an reasonably large (yet, odd) number of electrons.

Other examples of the potentially advantageous many-body correlations that can provide for massive pairwise as well as multi-party entanglement, include such phenomena as interaction-induced electron spin polarization, singlet Cooper pairing, Kondo screening of magnetic impurities, and dissipationless Quantum Hall states.

The main obstacles on the way of implementing quantum protocols has so far been and still remains a virtually unavoidable environmentally induced decoherence. The list of the previously discussed decoherence suppression/avoidance techniques contains such proposals as error correction (including the automatic one through dissipative evolution), encoding into decoherence-free subspaces, dynamical decoupling/recoupling schemes (e.g., "bang-bang" pulse sequences), and the use of the quantum Zeno effect.

However, none of the above recipes are entirely universal and their actual implementation may be hindered by such factors as a significant encoding overhead that puts a strain on the available quantum computing resources (error correction), a rather stringent requirement of a completely symmetrical qubits' coupling to the dissipative environment (decoherence-free subspaces) or a need for the frequency of the control pulses to be well in excess of the environment's bandwidth (dynamical decoupling/recoupling) or for a high precision continuous measurement (quantum Zeno effect).

Report Documentation Page				Form Approved OMB No. 0704-0188	
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE <b>20 FEB 2005</b>		2. REPORT TYPE <b>N/A</b>		3. DATES COVERED <b>-</b>	
4. TITLE AND SUBTITLE <b>Quantum Entanglement and Coherence of Electronic States in Nanoscale Devices</b>				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) <b>U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211</b>				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT <b>Approved for public release, distribution unlimited</b>					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT <b>SAR</b>	18. NUMBER OF PAGES <b>9</b>	19a. NAME OF RESPONSIBLE PERSON
a. REPORT <b>unclassified</b>	b. ABSTRACT <b>unclassified</b>	c. THIS PAGE <b>unclassified</b>			

While being more feasible in some (most notably, liquid-state NMR and trapped-ion) as compared to other quantum computing designs, the implementation of the above approaches is going to be particularly challenging in solid-state architectures. For one thing, any realistic prototype of a solid-state quantum register is going to be an assembly of a large number of physical qubits whose couplings, instead of being switchable on and off upon demand, will likely to have permanent (possibly, different for different pairs of qubits) components. In contrast to the liquid-state NMR and trapped-ion designs, in solid-state implementations of quantum information processing the practical possibilities of both, elimination of any stray couplings between the qubits and such active noise-suppression techniques as dynamical decoupling/recoupling ("bang-bang" pulses) are likely to be rather limited.

It is for this reason that a physics-conscious engineering of robust multi-qubit systems and a systematic approach to choosing the optimal (coherence-wise) values of their microscopic parameters appears highly desirable.

In its most extreme form, this idea has been previously discussed in the context of topological qubits. However, such proposals require an enormous overhead in encoding, since they use a macroscopic number of physical qubits in order to represent a handful of logical ones whose number being related to the ground state degeneracy or, in the case of a 1D chain, to the number of its open ends (two). Besides, the nearly perfect isolation of the topological qubits from the environment can also make both the initialization of and read-out from such qubits rather problematic.

Nevertheless, in the work reported below we have shown that even significantly less ambitious (yet, more memory-efficient) methods of controlling coherence can be devised on the basis of the insight gained in such more established topics in many-body physics as the theories of quantum spin chains and Kondo-like impurities. In particular, we explored the possibility of thwarting decoherence by virtue of permanent (yet tunable) inter-qubit couplings that allow for a construction of supercoherent (albeit only partially protected) logical qubits.

## 1.2 Objectives

In view of the above and with an eye on the prospective solid-state implementations of quantum information processing, this ARO-supported project was aimed at:

- Proposing new and gaining a firm theoretical understanding of the previously discussed, many-body physics-based, mechanisms of suppressing decoherence and maintaining controlled entanglement in systems of many ( $10^3$ - $10^4$ ) coupled qubits.
- Developing a systematic approach to identifying the optimal regime(s) for creating and manipulating entanglement and maintaining coherence of coupled qubits during their idling periods, gate operations, and read-out measurements, also in the presence of generic (non-Ohmic, non-Markovian, non-Gaussian, and/or non-uniform) noisy environments.
- Assessing the feasibility of implementing our specific theoretical recommendations in and carry out a comparative analysis of different solid-state qubits and a variety of architectures. Ascertaining, on the basis of this insight, the most promising designs of a practical multi-qubit quantum register as well as the best implementations of various universal quantum gates and their combinations.

## 1.3 Methods of Research

Towards achieving the above goals, we carried out a formal mapping of the multi-qubit arrays in question onto spin-chain, quantum impurity, and other many-body models which had been shown to be amenable to various analytical techniques developed in the theory of complex systems, quantum chaos, and quantum control.

These unifying approaches are expected to be largely independent of the physical make-up of the constituent qubits, for as long as the system conforms to a theoretical description in terms of (pseudo)spin operators.

Further, in addition to the analytical approaches, we used evolutionary optimization algorithms for determining the optimal parameter regime(s) of operation and the sequences of universal gates implementing various quantum protocols.

## 2 Main Results

### 2.1 Control of coherence and entanglement in multi-qubit arrays

Any viable technique of a controlled creation of and a confident manipulation with entangled quantum states must be able to provide solutions of all the three pivotal problems: creating entangled states, probing their entanglement, and minimizing the influence of parasitic cross-correlation effects. Also, any theoretical proposal addressing entanglement production and detection should be implemented in the experimentally relevant situations and adapted to the layout of a concrete device. Achieving these goals requires one to develop new and advance the existing theoretical and computational tools for analyzing entanglement and (de)coherence in multi-qubit assemblies.

To that end, we have further exploited the recently discovered connections between quantum information and statistical mechanics of strongly correlated spin systems. This relationship (which was originally prompted by the idea of using electron or nuclear spins as physical qubits) appears to have a much greater potential, as far as the control of quantum entanglement and coherence in a broad class of systems amenable to the formal (pseudo)spin description.

In particular, the recent studies of finite one-dimensional systems of  $N \gg 1$  coupled qubits with the nearest-neighbor (in general, anisotropic) Heisenberg exchange couplings revealed the onset of massive shared entanglement (quantified by such measures as von Neumann entropy or concurrence), which is considered to be an important resource for quantum information processing, near any quantum critical point. At first sight, these findings seem to suggest that it might be advantageous to operate a qubit chain as a quantum register in its near-critical regime (if any). However, such a conclusion would be incomplete without determining just for how long such an entanglement can be retained in the presence of a realistic (noisy) environment and/or qubit imperfections and control errors.

#### 2.1.1 Entanglement and decoherence in 1D qubit chains

To this end, in [1] we addressed the problem of decoherence in near-critical 1D qubit systems and computed the decay rates of the shared entanglement in terms of the reduced density matrix, thus demonstrating that for a generic encoding the dephasing and relaxation rates tend to increase dramatically as the system approaches the critical regime. These findings imply that the conditions

for achieving maximal sustainable entanglement and minimal decoherence turn out to be rather complementary (if not totally contradictory) with respect to each other. Therefore, it is conceivable that in order for a practical quantum computer to achieve the target performance in terms of both the degree of entanglement and reliable coherence control, rather significant trade-off has to be made.

Moreover, in Ref.[1], we showed that the "always-on" inter-qubit couplings destroy the conventional decoherence free Hilbert subspace present in the case of a non-interacting system subjected to a collective noisy environment. Instead we found some indications in favor of the possibility of using the multi-spinon basis for constructing "super-coherent" (albeit, not completely decoherence-free) Hilbert subspaces. A proof of the existence of such subspaces and the corresponding encoding schemes for creating robust logical qubits would represent a major breakthrough.

### 2.1.2 Flying qubits in 1D qubit chains

In [2] we put forward the idea that propagating spin-1/2 ("spinon") excitations provide a natural implementation of the notion of "all-spin" flying qubits. Unlike such previously discussed candidates as photons and ballistic electrons, spinons require no conversion from optical to spin degrees of freedom and produce no excessive heat (and/or noise) when they propagate through the qubit system. Further, we carried out a preliminary analysis of decoherence and entanglement properties of generic (non-integrable and/or disordered) multi-qubit chains that support all-spin flying qubits.

Alongside the onset of massive shared entanglement and/or qubit localization in the near-critical or diffusive regime, respectively, the decoherence rates (due to both external noise and qubits' cross-talk) were found to increase as the system is tuned towards criticality and/or localization. Moreover, we demonstrated that ordered, spin-isotropic, non-critical systems can better support and faithfully transmit robust flying qubits.

## 2.2 Robust qubits and optimal design of universal gates

Making a progress towards building a practical quantum register requires a firm theoretical understanding of the optimal conditions for suppressing decoherence and maintaining controlled entanglement in systems of many coupled qubits during their idling periods, gate operations, and read-out measurements, also in the presence of generic (non-Ohmic, non-Markovian, non-Gaussian, and/or non-uniform) environments.

A generic multi-qubit system in question is represented by the spin-boson Hamiltonian of  $N$  interacting qubits exposed to a dissipative environment

$$H(t) = \sum_{a,i} S_i^a (B^a(t) + \gamma^a h_i^a) + \sum_{a,i,j} I_{ij}^a(t) S_i^a S_j^a + \sum_k \omega_k b_k^\dagger b_k \quad (1)$$

An arbitrary quantum computing protocol consists of a sequence of short pulses implementing various one- ( $B_i^a(t)$ ) and two- ( $J_{ij}^a(t)$ ) qubit gate operations, whereas the qubit "cross-talk" described by either short-ranged (such as exchange,  $J_{ij}^a \propto \exp(-\text{Const}|i-j|)$ ), or long-ranged (such as dipolar,  $J_{ij}^a \propto 1/|i-j|^3$ ) couplings is present throughout the entire process of computation.

The random field  $h_i^a = \sum_k e^{i\vec{k}\vec{r}_i} \lambda_k^a (b_k^\dagger + b_{-k}) / \sqrt{\omega_k}$  represents the worst-case ((sub)Ohmic and, in general, non-uniform and/or multi-component) bosonic bath governed by the correlation function  $\langle h_i^a(t) h_j^b(0) \rangle \propto \delta^{ab} \Lambda^\epsilon / [t^2 - (R/v)^2]^{1-\epsilon/2}$ , where  $R = |i-j|$  is the distance between the  $i^{\text{th}}$  and  $j^{\text{th}}$

qubits and  $\Lambda$  is an upper cutoff of order the bath's bandwidth. The variable parameter  $0 < \epsilon < 1$  also controls the bath's spectral density  $\rho(\omega) = \sum_k (|\lambda_k^q|^2 / \omega_k) \delta(\omega - \omega_k) \propto \Lambda^\epsilon \omega^{1-\epsilon}$ , thus allowing one to study different (sub)Ohmic environments within the same unifying framework.

### 2.2.1 Many-body physics-conscious engineering of noisy environments

In Ref.[3] we demonstrated that the recent generalizations of the conventional Kondo problem known as the Bose- and Bose-Fermi Kondo models (originally developed in the theory of (non)magnetic impurities embedded in various heavy fermion and high- $T_c$  compounds) can be of a prime relevance to the problems involving qubits that are simultaneously subject to both Ohmic and non-Ohmic noise sources. Moreover, this formalism allows one to study the effects of non-Markovian and/or structured environments.

The formal analogy established in [3] enabled us to formulate a number of concrete recommendations for achieving the optimal (coherence-wise) regime for operating a noisy multi-qubit quantum register, such as the requirement of a spin-rotational invariance of the qubit-bath coupling that was found to guarantee the best possible conditions for preserving coherence.

As another important inference, in [3] we observed that one can improve the performance of a two-qubit register by tuning the inter-qubit coupling  $I$  (of the fixed, Heisenberg, symmetry) close to (yet, smaller than) the critical value  $I_*$  of the two-impurity Kondo model, thereby causing an incipient singlet formation and quenching of the individual Kondo screening.

### 2.2.2 Robust two-qubit registers

In Ref.[4] we demonstrated that the properly chosen permanent qubits' couplings do provide an additional layer of protection against decoherence. Specifically, in [4] we focused on the problem of preserving an arbitrary initial state ("quantum memory") of a basic two-qubit register during its idling period between consecutive gate operations.

The previous analyses of the problem in question have been largely limited to the range of parameter values corresponding to the presently available experimental setups. As a result, they have not systematically addressed a possible role of the inter-qubit couplings in reducing decoherence.

In [4] we studied the worst-case scenario of two uncorrelated ( $\langle h_1(t)h_2(0) \rangle = 0$ ) dissipative reservoirs and the configurations of the inter-qubit couplings that provide for the strongly reduced decoherence rates during both idling periods and elementary gate operations were identified. The analytical results were also confirmed with the use of genetic algorithms.

### 2.2.3 Single-step implementation of universal gates

In [5] we further exploited the findings of Ref.[4] in order to optimize the implementation of the universal quantum gates. Unlike in the previous proposal, we found significantly improved (shorter time, higher fidelity) implementations of a number of popular gates which can all be performed in a single step under the condition of degeneracy between the instantaneous energy levels.

A systematic search of the optimal sequences of operations implementing various universal gates and their combinations was carried out with the use of analytical approaches and numerical genetic

algorithms. The results of this analysis were applied to some of the previously proposed superconducting architectures of a functional quantum register subject to various realistic environments (Nyquist noise, localized two-level systems, phonons, etc.).

The rapid pace of a technological progress in solid-state quantum computing gives one a hope that the specific prescriptions towards building robust qubits and their assemblies made in the course of this work can be implemented in future devices. In this regard, particularly promising appear to be the phase, charge and charge-phase superconducting qubit architectures where, in principle, any desired symmetry of the interaction terms in the Hamiltonian (1) can be achieved by merely combining the capacitive and inductive couplings.

### **2.3 Future directions and ongoing projects**

Despite the termination of the ARO support as of July 30, 2005, we are currently pursuing a number of related research topics that have emerged from the reported work and that explore various decoherence-suppressing effects of the strong many-body correlations. Among such prospective topics are the *d*-wave Josephson junction qubits, the fully microscopic theory of which was put forward in Ref.[6], the idea of taking advantage of the unique properties of excitons in semimetals [7] and compressible Quantum Hall states [8].

## **3 Practical applications and broader impact of reported research**

This project addressed a suite of related problems pertinent to the effects of strong correlations in functional nanostructures that are both fundamentally important and potentially capable of far-outreaching technological applications. Because of its innovative and inter-disciplinary nature, we believe that the reported work has further advanced the ongoing process of cross-fertilization between the theory of quantum information and nanoscience.

Also, we believe that this project has complemented the existing ARO-funded experimental programs at UNC-Chapel Hill and helped to foster new collaborations. The home institution of this project, UNC-Chapel Hill, with its strong long-time commitment to research and education has provided an excellent environment for postdoctoral and student training.

The results obtained in the course of this work have been broadly disseminated through publications (see Refs.[1-8]) and presentations at a number of conferences and meetings (see Refs.[9-17]). We believe that these results have contributed towards the advancement of knowledge and further strengthened the case for utilizing the unique properties of strongly correlated condensed matter systems for constructing practical quantum computing devices.

## 4 References

### 4.1 Papers published in refereed journals

- [1] D. V. Khveshchenko, *Decoherence of one-dimensional flying qubits due to their cross-talk and imperfections*, Phys. Rev. **B70**, 092407 (2004).
- [2] D.V.Khveshchenko, *Quantum impurity models of noisy qubits*, Phys. Rev. **B69**, 153311 (2004).
- [3] D.V.Khveshchenko, *Entanglement and decoherence in near-critical qubit chains*, Phys. Rev. **B68**, 193307 (2003).
- [4] D. V. Khveshchenko and A. V. Grigorenko, *Single-step implementation of universal two-qubit gates*, Phys. Rev. Lett.**95**, 110501 (2005).
- [5] D. V. Khveshchenko and A. V. Grigorenko, *Robust two-qubit quantum registers*, Phys. Rev. Lett. **94**, 040506 (2005).

### 4.2 Papers submitted

- [6] D. V. Khveshchenko, *Dissipative dynamics of planar d-wave Josephson junctions*, submitted to Phys. Rev. Lett. (July 2005).
- [7] D. V. Khveshchenko and W. Shively, *Excitonic pairing between nodal fermions*, to be submitted to Phys. Rev. B.

### 4.3 Refereed book chapter

- [8] D.V.Khveshchenko and S.Washburn, *Phase coherence in mesoscopic systems at high magnetic fields*, in "High Magnetic Fields: Science and Technology", Eds. F.Herlach and N.Miura, (World Scientific, 2003).

### 4.4 Unpublished conference presentations

- [9] D. V. Khveshchenko and A. V. Grigorenko, *Optimized design of universal two-qubit gates*, Gordon Research Conference (Ventura, Feb. 2005).
- [10] D. V. Khveshchenko and A. V. Grigorenko, *Theoretical studies of robust two-qubit quantum registers*, Gordon Research Conference (Ventura, Feb. 2004).
- [11] D. V. Khveshchenko, *Interacting multi-qubit arrays*, Second Feynman Festival (University of Maryland, Aug. 2004).
- [12] D. V. Khveshchenko, *Many-body effects in multi-qubit systems*, Conference on Strongly Correlated Electrons (Brookhaven National Laboratory, Sep. 2003).
- [13] D. V. Khveshchenko, *Coherence control in multi-qubit systems*, Quantum Computing Program meeting (Washington DC, Feb. 2004).
- [14] D. V. Khveshchenko, *Entanglement and decoherence in multi-qubit systems*, Quantum Computing Program meeting (Harpers Ferry, May 2003).



## **4.5 Technical reports submitted to ARO and released on CD**

- [15] D. V. Khveshchenko, Progress report (Nashville, Aug. 2002).
- [16] D. V. Khveshchenko, Progress report (Nashville, Aug. 2003).
- [17] D. V. Khveshchenko, Progress report (Orlando, Aug. 2004).

## **5 Personnel supported by the Contract**

1. Dr D. V. Khveshchenko, PI (April 2002-June 2005);
2. Dr A. V. Grigorenko, Postdoctoral Associate (Aug. 2003-Feb. 2005);
3. Dr A. I. Yashenkin, Postdoctoral Associate (April 2002-Dec. 2002);
4. Mr R. Crooks, Graduate Student (May-June 2005).